

# The complement: a solution to finite size effects in phase transitions of nuclei and other mesoscopic systems

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In the case of liquid-vapor phase coexistence, a dilute nearly ideal vapor phase is in equilibrium with a dense liquid-like phase. The interesting case of finiteness is realized when the liquid phase is a finite drop. We introduce the concept of the complement (the residual drop which remains after a cluster has been emitted) in order to quantify finite size effects and to generalize the theory for cluster yields from extremely small systems. The complement approach consists of evaluating the change in free energy occurring when a particle or cluster is moved from one (finite) phase to another.

In order to demonstrate the power of this method, we apply it to the canonical lattice gas representation of the Ising model [1]. We fix the mean density of occupied sites so that below the coexistence temperature there is a large cluster in equilibrium with its vapor.

Fisher's theory of clusterization assumes that the monomer-monomer interaction exhausts itself in the formation of physical clusters in equilibrium with the liquid and themselves. The cluster concentration is given as

$$\begin{aligned} n_A(T) &= g(A) \exp\left(-\frac{c_0 A^\sigma}{T}\right) \\ &= q_0 A^{-\tau} \exp\left(c_0 A^\sigma \left[\frac{1}{T_c} - \frac{1}{T}\right]\right) \end{aligned} \quad (1)$$

where  $c_0 A^\sigma$  is the surface energy and  $g(A)$  is the cluster degeneracy and is approximately  $A^{-\tau} \exp(c_0 A^\sigma / T_c)$ . The resulting surface entropy  $S(A)$  is given by

$$S(A) \approx \ln g(A) \approx -\tau \ln A + \frac{c_0 A^\sigma}{T_c}. \quad (2)$$

Eq. (2) is a remarkably felicitous asymptotic expansion. The presence of a leading term in  $S$  proportional to  $A^\sigma$  permits the vanishing of the cluster free energy at a  $T = T_c$  independent of cluster size. This expression, valid for a vapor in equilibrium with the infinite liquid, must be generalized for equilibrium with a finite liquid.

For each cluster of the vapor we can make the mental exercise of extracting it from the liquid, determining the change in entropy and energy of the drop and cluster system, and then putting it back in the liquid (the equilibrium condition), as if all other clusters of the vapor did not exist. Fisher's expression can be written for a drop of size  $A_0$  in equilibrium with its vapor as follows

$$\begin{aligned} n_A(T) &= \frac{g(A)g(A_0 - A)}{g(A_0)} \\ &\exp\left\{-\frac{c_0}{T} [A^\sigma + (A_0 - A)^\sigma - A_0^\sigma]\right\} \end{aligned} \quad (3)$$

or

$$n_A(T) = q_0 \left[ \frac{A(A_0 - A)}{A_0} \right]^{-\tau}$$

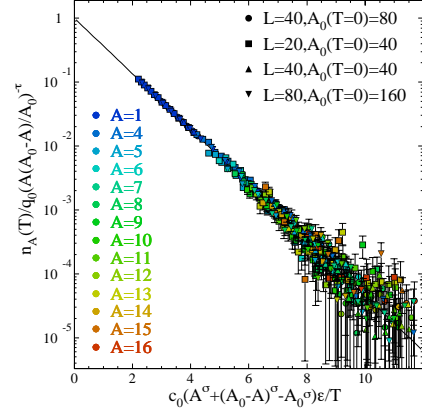


FIG. 1: The scaled cluster yields as a function of the surface energy with the complement for different combinations of lattice size  $L$  and mean density  $\rho$ .

$$\exp\left\{[A^\sigma + (A_0 - A)^\sigma - A_0^\sigma] \left(\frac{c_0}{T_c} - \frac{c_0}{T}\right)\right\}. \quad (4)$$

We treat the “complement”  $(A_0 - A)$  in the same fashion as a cluster. The resulting expression reduces to Eq. (1) when  $A_0 \rightarrow \infty$ . While different than the standard Fisher expression, Eq. (4) admits the **same**  $T_c$  as that of the infinite system. This is because the  $A_0, A$  dependence of the surface energy finds its exact counterpart in that of the surface entropy.

Our generalized form of the Fisher expression (Eq. (4)) can be used to fit vapor concentrations in equilibrium with a finite droplet. We can then examine a Fisher-like scaling plot of all the  $n_A(T)$ . Given Eq. (4) we can use any drop size and automatically correct for it by plotting  $\frac{n_A(T)}{\left(\frac{A(A_0 - A)}{A_0}\right)^{-\tau}}$  versus  $c_0(A^\sigma + [A_0 - A]^\sigma - A_0^\sigma)(1/T_c - 1/T)$ . This is shown in Fig. 1 for a variety of vapors in equilibria with drops of different sizes. The accurate scaling that is observed vouches for the generality of Eq. (4). The value of the critical temperature extracted is  $T_c = 2.28 \pm 0.02$ . This is to be compared with the theoretical value of  $2/\ln(1 + \sqrt{2}) = 2.26919\dots$  for the Ising model in two dimensions. One can now sum the Fisher concentrations of Eq. (4) to calculate the pressure and density of the vapor in coexistence with a given ground state droplet.

[1] T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410 (1952).